

Effective Range Corrections to Three-Body Recombination for Atoms with Large Scattering Length

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(Dated: February 3, 2008)

Few-body systems with large scattering length a have universal properties that do not depend on the details of their interactions at short distances. The rate constant for three-body recombination of bosonic atoms of mass m into a shallow dimer scales as $\hbar a^4/m$ times a log-periodic function of the scattering length. We calculate the leading and subleading corrections to the rate constant which are due to the effective range of the atoms and study the correlation between the rate constant and the atom-dimer scattering length. Our results are applied to ^4He atoms as a test case.

PACS numbers: 03.75.Nt, 34.50.-s, 21.45.+v

Keywords: three-body recombination, large scattering length, effective range corrections

A. Introduction

The properties of low-energy bosons are dominated by S-wave interactions. If the interaction is short ranged, these properties can be parametrized by the effective range expansion. The typical range of the interaction also defines a natural low-energy length scale l [1]. For a finite range potential l is simply given by the range of the potential. If the potential has a van der Waals tail $-C_6/r^6$, it is determined by the van der Waals length $l_{vdW} = (mC_6/\hbar^2)^{1/4}$, where m is the mass of the bosons. For a generic physical system, the effective range parameters, such as the scattering length a and the effective range r_e , are of the same order of magnitude as l . In some systems, however, the scattering length a is much larger than l while the effective range $r_e \sim l$ is still of the same order of magnitude. This situation requires a fine tuning of the parameters in the underlying potential. Typical examples are ^4He atoms and nucleons where this fine tuning is accidental, or alkali atoms near a Feshbach resonance where it can be controlled experimentally by changing an external magnetic field.

Physical systems with large $|a|$ display a number of

interesting effects and universal properties that are independent of the details of the interaction at short distances of order l [1]. The simplest example for positive a is the existence of a shallow two-body bound state (called a dimer) with universal binding energy $B_2 = \hbar^2/(ma^2)[1 + \mathcal{O}(l/a)]$. Similar relations hold for other observables, which can generally be described at low energies by a controlled expansion in $l/|a|$. Particularly interesting is the structure of the three-boson system. It has universal properties that include a geometric spectrum of three-body bound states (so-called Efimov trimers), log-periodic dependence of three-body observables on the scattering length, and a discrete scaling symmetry [2, 3, 4]. These properties can be studied using effective theories which provide a powerful framework to exploit the separation of scales between a and l [1, 5, 6].

Since we are mainly interested in applications to atomic systems, we will refer to the bosons as atoms in the following. In particular, we focus on three-body recombination, the process in which three atoms collide to form a diatomic molecule and an atom. The energy released by the binding energy of the molecule goes into the kinetic energies of the molecule and the recoiling atom. If the momenta of the incoming atoms are sufficiently small compared to $1/a$, the momentum dependence of the recombination rate can be neglected. The recombination event rate constant α is defined such that the number of recombination events per time and per volume in a

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gas of cold atoms with number density n_A is αn_A^3 . If the atom and the dimer produced by the recombination process have large enough kinetic energies to escape from the system, the rate of decrease in the number density of atoms is

$$\frac{d}{dt}n_A = -3\alpha n_A^3. \quad (1)$$

For large positive a , recombination can go into the shallow dimer with binding energy $B_2 = \hbar^2/ma^2$ and another atom. If no deep dimers are present, this is the only channel for recombination to occur. Three-body recombination into deep dimers can also be treated using similar methods [1, 7, 8, 9]. However, here we assume that no deep dimers are present. We focus on $a > 0$ and consider 3-body recombination into the shallow dimer.

B. Theoretical framework

We first briefly review the universal expressions at leading order in the expansion in l/a . Dimensional analysis together with the discrete scaling symmetry implies that α is proportional to $\hbar a^4/m$ with a coefficient that is a log-periodic function of a with period π/s_0 . To very high accuracy, the three-body recombination constant α can be expressed as [9, 10, 11]:

$$\alpha = 67.12 \sin^2(s_0 \ln(a/a_*) + 1.67) \frac{\hbar a^4}{m} [1 + \mathcal{O}(l/a)], \quad (2)$$

where $s_0 = 1.00624\dots$ is a transcendental number and a_* is the scattering length at which there is an Efimov trimer at the atom-dimer threshold. Note also that an analytic expression for the coefficient 67.12 has recently been derived [12, 13]. The most remarkable feature of the expression in Eq. (2) is that the coefficient of $\hbar a^4/m$ oscillates between zero and 67.12 as a function of $\ln(a)$. In particular, α has zeroes at values of a that differ by $e^{\pi/s_0} \approx 22.7$. The locations of these zeros can be expressed as $a \approx (e^{\pi/s_0})^n 0.20 a_*$ where n is an integer. The maxima of α/a^4 occur at $a \approx (e^{\pi/s_0})^n 0.94 a_*$. These maxima are close to the values $a = (e^{\pi/s_0})^n a_*$ for which there is an Efimov trimer at the atom-dimer threshold. In the latter case, atom-dimer scattering becomes resonant and the atom-dimer scattering length diverges.

At leading order in l/a , the atom-dimer scattering length can be expressed as [1, 4]:

$$a_{ad} = (2.15 \cot(s_0 \ln(a/a_*)) + 1.46) a [1 + \mathcal{O}(l/a)]. \quad (3)$$

Solving Eq. (3) for a_* , we can eliminate a_* from Eq. (2) and obtain an analytical expression for the universal correlation between α and a_{ad} . In this paper, we study the correlation between α and a_{ad} up to second order in the expansion in l/a . To this order, these corrections are fully determined by the S-wave effective range r_e [14]. Therefore, we refer to them as effective range corrections.

The quantities α and a_{ad} can both be calculated from the following integral equation:¹

$$\mathcal{A}_S(p, k; E) = \frac{16\pi\gamma}{1 - \gamma r_e} V(p, k; E) + \frac{4}{\pi} \int_0^\Lambda dq V(p, q; E) \times \frac{q^2 \mathcal{A}_S(q, k; E)}{-\gamma + (\frac{3}{4}q^2 - E - i\epsilon)^{1/2} - \frac{1}{2}r_e(\frac{3}{4}q^2 - E - \gamma^2)}, \quad (4)$$

where Λ is an ultraviolet cutoff, r_e is the effective range, and γ denotes the position of the bound state pole in the atom-atom Green's function:

$$\gamma = \left(1 - \sqrt{1 - 2r_e/a}\right) \frac{1}{r_e}, \quad (5)$$

where we have set $\hbar = m = 1$ for convenience. The potential $V(p, k; E)$ is

$$V(p, k; E) = \frac{1}{2pk} \ln \left(\frac{p^2 + pk + k^2 - E}{p^2 - pk + k^2 - E} \right) + G_3(\Lambda), \quad (6)$$

where $G_3(\Lambda)$ represents the contribution from the contact three-body interaction. For $r_e = 0$, it is given by [5, 6]

$$G_3(\Lambda) \approx \frac{1}{\Lambda^2} \cot(s_0 \ln(\Lambda a_*) + 2.45), \quad (7)$$

but for finite effective range its form is more complicated. In the following, we will directly calculate the correlation between α and a_{ad} , therefore a_* will not explicitly appear. In our case of positive a , γ^2 is the binding energy of the shallow dimer. At leading order (LO) in l/a , γ reduces to $1/a$ but the two quantities differ if the effective range is included. We have chosen γ and r_e as our 2-body inputs instead of a and r_e , because this choice keeps the location of the dimer pole fixed which leads to a faster convergence of the effective-range expansion. The effective theory expansion is then in powers of γl .

From the general solution of Eq. (4) one can directly obtain α and a_{ad} . The three-body recombination constant α is given by

$$\alpha = \frac{8}{\gamma^2 \sqrt{3}} \frac{(1 - \gamma r_e)}{(1 - \gamma r_e/2)^2} \left| \mathcal{A}_S(0, 2\gamma/\sqrt{3}; 0) \right|^2, \quad (8)$$

while the atom-dimer scattering length is given by

$$a_{ad} = -\frac{1}{3\pi} \mathcal{A}_S(0, 0; -\gamma^2). \quad (9)$$

In principle one can obtain the effective range corrections to all orders by solving the integral equation in Eq. (4) directly. A potential problem comes from the dimer propagator in the second line of Eq. (4). In addition to the pole from the shallow dimer with $\gamma \sim 1/a$, it

¹ For a derivation of this equation from effective field theory, see e.g. Ref. [1].

also has a deep pole with $\gamma \sim 1/r_e$. This pole is an artefact of the form of the dimer propagator and is outside the range of validity of the effective theory. For negative effective range, the pole is on the unphysical sheet of the complex momentum plane and causes no problems in solving Eq. (4). For positive effective range, the pole is on the physical sheet and leads to instabilities in the three-body equations for cutoffs of the order $\sim 1/r_e$ and larger. We avoid this problem by expanding the kernel of Eq. (4) in the effective range r_e and solving the resulting integral equation. This allows to calculate the range corrections perturbatively up to order $(\gamma l)^2$. For higher orders, things become more complicated and a new three-body parameter enters [14]. Moreover, for particles with an interaction displaying a van der Waals tail $\sim C_6/r^6$, the true interaction can only be approximated by contact interactions up to order $(\gamma l)^2$. If a higher accuracy is required, the van der Waals tail has to be taken into account explicitly [1]. For positive effective range, we performed all calculations with a cutoff well above the breakdown scale of the theory $\Lambda \gg 1/r_e$. For negative effective range the calculation at next-to-leading order (NLO) has to be performed with cutoffs $\Lambda \sim 1/r_e$. This is due to a cancellation between even and uneven orders in the expanded two-body propagator at values of the loop momentum $q \gg 1/r_e$ [14]. In uneven orders of the expansion in r_e this would lead to an incorrect renormalization if the cutoff was taken much larger than $1/r_e$. In next-to-next-to-leading order (NNLO), the term proportional to $(\gamma r_e)^2$ dominates the expansion of the two-body propagator for large loop momenta and the problem is not present.

We calculate the effective range corrections to the correlation between α and a_{ad} two different ways: (i) in the subtractive renormalization scheme of Ref. [14] where the three-body force term $G_3(\Lambda)$ does not explicitly appear and (ii) by performing a calculation at fixed cutoff Λ and varying G_3 .² Both methods agree to very high precision.

C. Correlation between α and a_{ad}

The results for the correlation between α and a_{ad} for positive effective range $r_e > 0$ are shown in Fig. 1 for two different values of the effective range. The solid line gives the leading order result, while the dashed and dash-dotted lines give the NLO and NNLO results, respectively. The light (dark) curves are for $\gamma r_e = 0.1$ ($\gamma r_e = 0.3$). For large absolute values of a_{ad} and $\gamma r_e = 0.1$ the shift from LO to NLO is accidentally very small. However, the shift from NLO to NNLO is of the expected size of $(\gamma r_e)^2 \sim 0.01$ and is larger than from LO to NLO. A similar observation holds for the case

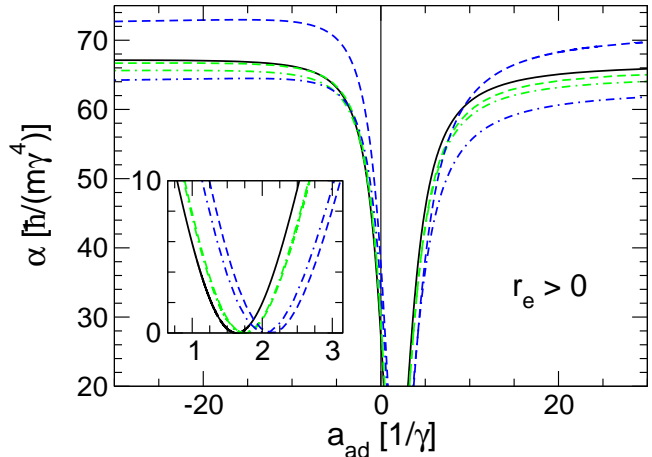


FIG. 1: Correlation between α and a_{ad} for $r_e > 0$. The solid line gives the leading order result, while the dashed (dash-dotted) lines give NLO (NNLO). The light (dark) curves are for $\gamma r_e = 0.1$ ($\gamma r_e = 0.3$).

$\gamma r_e = 0.3$. We observe that the shift from LO to NLO varies strongly in size and is sometimes smaller than expected by naive dimensional analysis. However, the shift from NLO to NNLO is generally of the expected order of magnitude. The smallness of the NLO corrections can be understood as a cancellation between two different contributions to this correction. The two contributions are proportional to γr_e and κr_e , respectively, where κ is the typical momentum scale of the process. Furthermore, it is known from experience [1] that at LO observables are often described better than expected from the power counting once the exact pole position of the two-body propagator is reproduced. As a consequence, the shifts in observables from LO to NLO can be very small and of a size comparable to the corresponding shifts from NLO to NNLO. The minimum in the correlation curve is moved to larger values of a_{ad} . The size of this shift is of the order γr_e from LO to NLO, and of the order $(\gamma r_e)^2$ from NLO to NNLO.

We emphasize that an error estimate determined by the truncation error of the EFT expansion can be given from dimensional analysis within the EFT approach. However, this does not necessarily imply that the shift from one order to the next has to be exactly equal to this error estimate. Firstly, the error estimate is only accurate up to a number of $\mathcal{O}(1)$ which depends on the details of the problem and cannot be estimated *a priori*. Secondly, if there are competing dynamical contributions at a given order, cancellations may lead to significantly smaller corrections as can be seen in our results.

The results for the correlation between α and a_{ad} for negative effective range $r_e < 0$ are shown in Fig. 2 for two different values of the effective range. Again, the solid line gives the leading order result, while the dashed and dash-dotted lines give the NLO and NNLO results,

² Since proper renormalization has been explicitly verified, practical calculations can be carried out at fixed cutoff Λ .

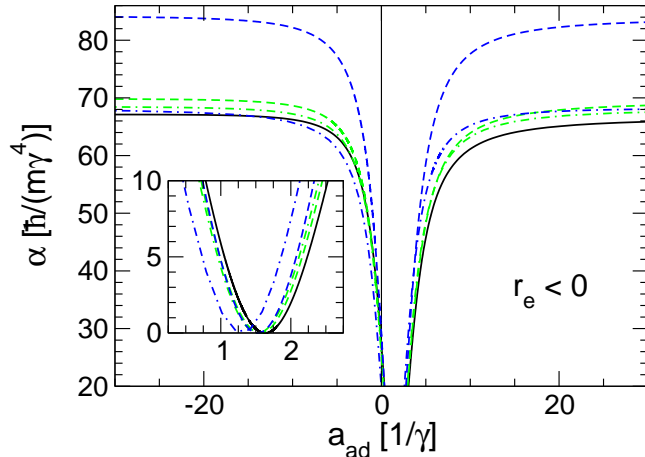


FIG. 2: Correlation between α and a_{ad} for $r_e < 0$. The solid line gives the leading order result, while the dashed (dash-dotted) lines give NLO (NNLO). The light (dark) curves are for $\gamma r_e = -0.1$ ($\gamma r_e = -0.3$).

respectively. The light (dark) curves are for $\gamma r_e = -0.1$ ($\gamma r_e = -0.3$). For $\gamma r_e = -0.1$, we find that the corrections scale as expected. In the case $\gamma r_e = -0.3$, the behavior at NNLO resembles the case for positive effective range. The minimum is shifted to smaller values of a_{ad} . From LO to NLO the size of the corresponding shift is of the order γr_e and from NLO to NNLO it is approximately of the order $(\gamma r_e)^2$.

For negative effective range, the maximum value of $\alpha m \gamma^4 / \hbar$ in NLO is very sensitive to the value of r_e , while at NNLO this sensitivity disappears and the maximum value is close to the LO result. For $r_e > 0$, the sensitivity persists at NNLO. It is also evident that the convergence of the EFT expansion may be slow for large absolute values of a_{ad} . For smaller $|a_{ad}|$, rapid convergence can be achieved for larger values of γr_e . Indeed it will be shown below that for ^4He atoms the encountered values of γr_e are well within the range of applicability of the EFT expansion. The correlation curve has a pronounced minimum and is not completely symmetric around this minimum value which lies in the interval $1 < \gamma a_{ad}^{\min} < 2$. As a consequence, there will always be 2 solutions for a_{ad} if α is used as three-body input.

D. Application to ^4He atoms

As an illustration, we apply our results to ^4He atoms for which the condition $\gamma l \ll 1$ is well satisfied [1, 15, 16]. The interatomic potential between two ^4He atoms does not support any deep dimers, such that our calculations are applicable. The binding energies of the ^4He trimers have been calculated accurately for a number of different model potentials for the interaction between two ^4He atoms. (See, e.g., Refs. [17, 18, 19] and references

therein.) The ^4He dimer and trimer ground states have been observed in experiment [20, 21], but the excited state of the trimer has not yet been seen. Due to the limited experimental information in the three-body sector, we apply our effective theory to the TTY [22] and HFD-B3-FCI1 [25] potentials. The input parameters for the effective theory are the dimer binding energy and the effective range in the two-body sector plus one three-body observable. Once these parameters are specified, all other three-body observables can be predicted to NNLO in the EFT expansion. In the following, we use the effective theory to predict α if a_{ad} is known for a given potential and vice versa.

We consider first the TTY potential [22]. The scattering length for the TTY potential is $a = 100.01 \text{ \AA}$. This is much larger than its effective range $r_e = 7.329 \text{ \AA}$, which is comparable to the van der Waals length scale $\ell_{\text{vdW}} = 5.398 \text{ \AA}$ [1, 23]. The binding energy of the ^4He dimer for the TTY potential is $B_2 = 1.30962 \text{ mK}$ which is small compared to the natural low-energy scale for ^4He atoms: $E_{\text{vdW}} \approx 420 \text{ mK}$. This energy B_2 corresponds to a pole position $\gamma = 0.01040 \text{ \AA}^{-1}$. The atom-dimer scattering length for the TTY potential was calculated in Ref. [24] as $a_{ad} = (1.205 \pm 0.001)\gamma^{-1}$. Using this information as the three-body input and the effective range for the TTY potential, $r_e \gamma = 0.076$, we can obtain the recombination constant α which has not been calculated for the TTY potential. Our results are given in Table I.

TABLE I: Recombination constant α in units of $\hbar/(m\gamma^4)$ for the TTY potential [22]. The errors given correspond to the uncertainty in the input quantity a_{ad} . (Note that $\hbar^2/m = 12.1194 \text{ K \AA}^2$ for ^4He atoms.)

	LO	NLO	NNLO
$\alpha [\hbar/(m\gamma^4)]$	2.791 ± 0.013	3.899 ± 0.015	3.778 ± 0.014

The values are numerically accurate to the number of digits given. Even at NNLO the numerical errors in the input parameters are typically negligible compared to the truncation error of the effective theory. As an illustration, we have propagated the numerical error in the input parameter a_{ad} to the results in Table I. It should be emphasized that the physical accuracy is determined by the truncation error of the effective theory. The effective theory error estimates are 10%, 1%, and 0.1% times a number of $\mathcal{O}(1)$ at LO, NLO and NNLO, respectively. The actual difference between LO and NLO and NLO and NNLO in our results is 40% and 4%, respectively, but still in agreement with the above expectation. From this pattern we expect our NNLO result to be accurate to 0.4%. This slightly larger error than expected is due to the value of $\alpha m \gamma^4 / \hbar$ close to the minimum in the correlation curve, where small corrections are relatively more important. In Ref. [15], α was calculated at LO using the trimer excited state energy instead of a_{ad} as the three-body input and the value $\alpha = 2.9 \hbar/(m\gamma^4)$ was found. This result is in good agreement with our value at LO.

For the HFD-B3-FCI1 potential [25], the situation is the opposite and a_{ad} is unknown. However, the recombination constant $\alpha = 12 \cdot 10^{-29} \text{ cm}^6/\text{s}$ has been calculated [26]. The scattering length for this potential is $a = 91.0 \text{ \AA}$, which is again much larger than the effective range $r_e = 7.291 \text{ \AA}$ and the van der Waals length scale $\ell_{\text{vdW}} = 5.398 \text{ \AA}$ [1, 23]. The position of the dimer pole is $\gamma = 0.01149 \text{ \AA}^{-1}$. From this information, we can extract $r_e \gamma = 0.084$ and $\alpha m \gamma^4 / \hbar = 1.32$. Because of the shape of the curve in Fig. 1, we have now two solutions for a_{ad} as shown in Table II.

TABLE II: The two solutions for the atom-dimer scattering length a_{ad} in units of γ^{-1} for the HFD-B3-FCI1 potential [25]. (Note that $\hbar^2/m = 12.1194 \text{ K\AA}^2$ for ^4He atoms.)

	LO	NLO	NNLO
$a_{ad}[\gamma^{-1}]$ (solution 1)	1.341	1.434	1.424
$a_{ad}[\gamma^{-1}]$ (solution 2)	1.931	2.034	2.024

Using the information on a_{ad} from the TTY potential above, we can identify solution 1 as the appropriate one for ^4He atoms. The effective theory error estimates are 10%, 1%, and 0.1% times a number of $\mathcal{O}(1)$ at LO, NLO, and NNLO, respectively. In this case, the difference between LO and NLO as compared to the difference between NLO and NNLO is a factor of 0.7 smaller than the above estimate and thus in good agreement with the expectation. From this pattern we expect the error of our NNLO result to be 0.1 %. In Ref. [1], a_{ad} was calculated at LO using the trimer excited state energy instead of α as the three-body input and the value $\gamma a_{ad} = 1.4$ was found. Again, this result is in good agreement with our value at LO. The deviation between results using different three-body inputs gives a simple estimate of higher order corrections. For a_{ad} , this estimate works well. In the calculation of α discussed above, however, this estimate is misleading because the value of α is close to the minimum of the correlation curve.

E. Conclusions

In this work we have computed the effective range correction to the recombination coefficient α to second order in the expansion in γl . Up to this order, only the two-body scattering length a and effective range r_e plus one three-body parameter are required as input for the ef-

fective theory [14]. We have calculated the correlation between the atom-dimer scattering length a_{ad} and the recombination coefficient α at LO, NLO and NNLO, and studied the convergence of the effective theory expansion in γl . We found that the convergence of the EFT expansion may be slow for large absolute values of a_{ad} . For natural values $|\gamma a_{ad}| \lesssim 3$, rapid convergence could be achieved for $\gamma r_e \lesssim 0.3$. In the same manner, the correlation between α and other low-energy three-body observables, such as Efimov trimer energies, could be calculated. As a test, we have applied our results to ^4He atoms. We have used the TTY [22] and HFD-B3-FCI1 potentials [25] as input and predicted, using the effective theory, three-body observables that have not yet been calculated for these potentials. The convergence of the expansion in γl for ^4He atoms was found to be in agreement with the *a priori* expectation.

Further efforts should be devoted to the inclusion of effective range corrections for recombination processes in ultracold gases of alkali atoms. Such atoms have many deep two-body bound states which modify the recombination into the shallow dimer and provide additional channels for recombination into the deep states. At LO in the expansion in γl these effects have already been calculated in this effective theory [1, 7, 8, 16]. An extension to NNLO and the inclusion of temperature dependence (see Refs. [27, 28, 29]) should allow for a precise description of experimental loss rates such as obtained by the Innsbruck group for ^{133}Cs atoms [30]. The recombination of cold helium atoms at nonzero collision energies has already been considered by Suno and coworkers [31]. A further step to increase the precision with which these experiments can be described theoretically is to include the recombination into Efimov trimers and dimer-dimer scattering resonances [32, 33]. Recent results in the four-body sector give hope that this goal can be achieved within the present effective theory framework [34, 35, 36].

Acknowledgments

This research was supported by the U.S. Department of Energy under grant DE-FG02-93ER40756 (LP) and DE-FG02-97ER41014 (TL), and by an Ohio University postdoctoral fellowship. We thank D.R. Phillips for discussions. LP thanks the theory group of the HSKP at Bonn University for its hospitality during the completion of this work.

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